Coefficient Adaptation Method for the Zwart Model

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(Received January 15, 2018; accepted July 3, 2018)

ABSTRACT

The coefficient adaptation problem is often encountered in CFD simulations. The accuracy of simulation results depends much on the empirical coefficients of mathematical models. Cavitation simulation is a typical application of CFD. Researchers have proposed methods to optimize the empirical coefficients of the cavitation model. However, these methods can only acquire constant values which aren’t adaptive to all the operating conditions. This paper focused on the condensation and the evaporation coefficients of the Zwart model and considered quasi-steady cavitating flows around a 2-D NACA66(MOD) hydrofoil. For the first time, we gave a formal description of the coefficient adaptation problem, and put forward a method to model the relationship between the best coefficient values and the operating conditions. We designed and implemented the coefficient adaptation platform combining OpenFOAM, and validated the best coefficient values predicted by our method. The overall results show the predicted coefficient values result in an increase of accuracy by 12% in average, compared with the default values and the tuned values by Morgut, thus indicating our method can effectively solve the coefficient adaptation problem for the Zwart model. We believe the proposed method can be extended to other mathematical models in practical uses.

Keywords: Coefficient optimization; Zwart model; OpenFOAM; Cavitation; CFD.

1. INTRODUCTION

Cavitation is the phenomenon that occurs inside a liquid medium or on the surface of liquid and solid medium with the process of formation, development and collapse of cavities (or bubbles). It is commonly observed inside or on the surface of fluid machinery such as water airfoils, hydraulic turbines, pumps and marine propellers. Due to the geometry of the system, cavitation appears in low pressure regions of the flowing liquids where local pressure drops below a certain threshold value. In these examples, the occurrence of cavitation is undesirable because it usually leads to negative effects such as vibration, noise and material erosion (Brennen 1995; Franc and Michel 2005). It is critical to study the mechanism of cavitation in order to reduce the losses in industrial applications.

With the fast development of computer techniques in the last few decades, CFD (Computational Fluid Dynamics) methods have been playing an increasingly important role in investigating cavitation because of less consumption of both time and resources compared to physical experiments. To describe the process of cavitation, researchers have developed numerous cavitation models, which can be divided into two categories, namely interface tracking models (Hirschi, Dupont, Avellan, Favre, Guelich, Handlower, and Parkinson 1998; Senocak and Wei 2004) and homogeneous equilibrium models (Merkle, Feng, and Buelow 1998; Kunz, Boger, Stinebring, Chyczewski, Lindau, Gibeling, Venkateswaran, and Govindan 2000; Schnerr 2001; Singhal, Athavale, Li, and Jiang 2002; Philip J. Zwart 2004). The former models are limited to two-dimensional planar or axisymmetric flows and difficult with three-dimensional simulation. The latter assume cavitating flows to be homogeneous and isothermal and solve the variation of the mixture density in the multiphase flow using a barotropic equation of state or a transport equation. However, barotropic equation of state cannot capture the dynamics of unsteady cavitating flows (Senocak and Shyy 2002); on the contrary, applying transport equations can simulate both steady and
unsteady cavitating flows. In the approach of transport equation models, an additional transport equation for either the mass or volume fraction of vapor with source terms to regulate the mass transfer between the two phases is solved. In the past decades, numerous transport equation models were proposed such as the Merkle model (Merkle, Feng, and Buelow 1998), the Kunz model (Kunz, Boger, Stinebring, Chyczewski, Lindau, Gibeling, Venkateswaran, and Govindan 2000), the Schnerr-Sauer model (Schnerr 2001), the Singhal model (Singhal, Athavale, Li, and Jiang 2002), the Zwart model (Philip J. Zwart 2004) and etc. They take into account different aspects of cavitating flows and imply different equations with evaporation and condensation rates to describe phase change. Most of these models include tunable parameters such as the condensation coefficient and the evaporation coefficient. Among them, the Zwart model has been integrated into commercial softwares such as ANSYS-CFX and fluent and widely used in simulating cavitating flows because of its effectiveness and stability (Philip J. Zwart 2004; Hagar Alm, Zhang, and Medhat 2012; Hou-lin, WANG, Deng-hao, Wei-min, and Ming-gao 2012).

The empirical coefficients of the cavitation models will affect the accuracy of simulation. Although default values of the coefficients are usually provided, they cannot always result in desirable simulation results. Thus, optimization of the empirical coefficients has to be performed. In recent years, researchers have investigated how to acquire better coefficient values. Hou-lin Liu et al. tested the value of each one of the four empirical coefficients of Zwart model by different orders of magnitude while setting the other three coefficients by default (Liu, Wang, Wang, Zhang, and Huang 2014). The results indicate the influence of each coefficient and the best order of magnitude for precise prediction. Morgut et al. tuned the empirical coefficients of the Zwart model, the Singhal model and the Kunz model respectively based on the simulation of the cavitating flow around the NACA66 (MOD) hydrofoil, using an optimization strategy driven by the modelFRONTIER optimization system, where three different cavitating flow regimes(different cavitation numbers) at the angle of attack of 4° were considered (Morgut, Nobile, Bilu, and Scaron 2011). The tuned coefficients agreed relatively well with the corresponding experiments of the three regimes and were then applied in the prediction of other flow regimes related to the NACA66 (MOD) hydrofoil. Surrogate-based optimization was also applied by some researchers to calibrate the coefficients in the simulation of some cavitating flows (Tushar, Siddharth, Haifka, Wei, and Zhao 2010; Zhao, Huang, Chen, Wang, Gao, and Zhao 2017). In literature efforts were made for the purpose of obtaining fixed values of the empirical coefficients that may generally go well with simulations under different operating conditions and even in new flow systems. It should be noted that fixed values cannot always perform well when operating conditions change. Meanwhile, in practical engineering, using traditional optimization method to find the best coefficient values will consume lots of time and resources. The above issues generate demand for efficient and intelligent coefficient recommendation methods that help with the prediction of the best coefficient values adapted to certain operating conditions. It is of great significance to discover the relationship between the best coefficient values and the operating conditions using intelligent methods when more and more experimental measurements under different operating conditions have been acquired.

Besides the cavitation model, the turbulence model also plays an important role in cavitation simulations. In literature, two common categories of the turbulence model have been proposed, namely Boussinesq-based eddy viscosity models and Reynolds stress models. The former category includes the zero-equation model, the Spalart-Allmaras model and the two-equation models. The other category introduces a control equation of second order pulsation to form the second order moment closed model (Wilcox 1993). In actual engineering, the Spalart-Allmaras model and the two-equation turbulence models are widely used. These models can save computation time as well as produce simulation results which meet with engineering requirements. Among these models, the standard k – ε model (Launder and Spalding 1974) is one of the earliest two-equation turbulence models. It has been proved to have good performance in simulating the steady-state cavitating flows around the two-dimensional NACA66(MOD) hydrofoil (Singhal, Athavale, Li, and Jiang 2002; Morgut, Nobile, Bilu, and Scaron 2011).

Aiming at the issue mentioned above, we focused on the Zwart model and carried out research into the prediction of the best values of empirical coefficients, considering quasi-steady cavitating flows around a two-dimensional NACA66 (MOD) hydrofoil. For the first time, we give a formal description of the coefficient adaptation problem and solution. We put forward the coefficient adaptation model and corresponding method including two key modules: the optimization module and the prediction module, which can model relationship between the best coefficient values and the operating condition-s. We designed and implemented the coefficient adaptation platform for the Zwart model through the method mentioned above, combining the open source software OpenFOAM. Then we performed optimization of the condensation coefficient Fc and the evaporation coefficient Fe of the Zwart model and validated the predicted optimal coefficient values on the platform. The overall results indicate that our method can effectively solve the coefficient adaptation problem of the Zwart model and guide the configuration of the empirical coefficients under specific operating conditions. It should be noted that our coefficient adaptation method is not limited to the Zwart model, but can be extended to other cavitation models or even other CFD models with empirical coefficients.
In the following, the formal description of coefficient adaptation problem is presented first, followed by the CFD models used in our simulations. Then the coefficient adaptation model for the Zwart model and the corresponding method are described. The experiments and numerical results are reported followed by our concluding remarks.

2. FORMAL DESCRIPTION OF COEFFICIENT ADAPTATION PROBLEM

The coefficient adaptation problem is that for the simulation of a specific flow case, how to decide the best values of empirical coefficients making the simulation results in best agreement with the experimental data for different operating conditions. Before giving our coefficient adaptation method, we present formal description of the coefficient adaptation problem. For a specific flow case Case, let \( D \) denote the calculating domain, \( M \) the mathematical models used to describe the flow, \( N \) the numerical methods involved in the simulation, \( I \) the initial conditions of the simulation, then the simulation results can be defined as:

\[
\text{Sim}_{\text{Case}}(O, M, N, I)
\]  

The initial conditions include the operating conditions and other initial settings. In later context, we replace \( I \) with \( O \) expressing the attention we pay to the operating conditions and neglect of other initial settings. \( M \) consists of several mathematical equations, each of them containing none or several empirical coefficients. Let the empirical coefficients be the independent variables, then the equations may take the form as:

\[
\begin{align*}
\text{Formula}_1(c_{11}, \cdots, c_{1p_1}) &= 0 \\
\text{Formula}_2(c_{21}, \cdots, c_{2p_2}) &= 0 \\
&\vdots \\
\text{Formula}_m(c_{m1}, \cdots, c_{mp_m}) &= 0
\end{align*}
\]  

(2)

Here, \( c_{11}, \cdots, c_{ip_i} \) are the empirical coefficients in the \( i \)th equation, and \( p_i \geq 0 \) (\( i = 1, \cdots, m \)). Specially, \( p_i = 0 \) means there is no coefficient in the \( i \)th equation. Let \( C = (c_{11}, \cdots, c_{1p_1}, \cdots, c_{m1}, \cdots, c_{mp_m}) \) represent the vector consisting of all the empirical coefficients, and \( M(C) \) denote the mathematical models \( M \) with the coefficients \( C \). Because the coefficient adaptation problem focuses only on the relationship between the coefficients \( C \) and the operating conditions \( O \), we simplify Eq. (1) as:

\[
\text{Sim}(M(C), O)
\]  

(3)

Let \( \text{Exp}_O \) denote the experimental data related to \( O \), then we define the distance between the simulation results and experimental data specifically for \( C \) and \( O \) as \( f_0(C) \) (which will be called the objective function from now on):

\[
f_0(C) = \left| \text{Sim}(M(C), O) - \text{Exp}_O \right|
\]  

(4)

Here, we redefine the combined meaning of the absolute value sign and the minus sign, representing a feasible way of calculating how far the simulation results deviate from the experimental data. Let \( C_{\text{Best}_O} \) denote the best values of coefficients under the operating conditions \( O \), then the formal description of coefficient adaptation problem can be given as:

\[
C_{\text{Best}_O} = \text{argmin}_{C} f_0(C)
\]  

(5)

We assume that the best values of the coefficients will change with the operating conditions, which can be described by a mathematical equation. Let \( C_{\text{Best}} = (c_{11}, \cdots, c_{cr}) \in \mathcal{C} \) denote the \( r \)-dimensional vector of all the coefficients, \( O = (o_1, \cdots, o_s) \in \mathcal{O} \) the \( s \)-dimensional vector consisting of \( s \) operating condition components, \( \mathcal{C} \subseteq \mathbb{R}^r, \mathcal{O} \subseteq \mathbb{R}^s \), then the equation can be written as:

\[
C_{\text{Best}} = g(O)
\]  

(6)

Here, \( g(O) \) is vector-valued with \( r \) components, and \( g \) represents a certain mapping rule from the domain \( \mathcal{O} \) to the domain \( \mathcal{C} \).

If such equation(s) shown in Eq. (6) is acquired, tedious work of simulation and calibration with experimental data before determining the best values of coefficients can be simplified. To the best of our knowledge, there exists no theory that demonstrate the relationship between the best values of coefficients and the operating conditions. Our idea is to analyze the potential relationship and figure out the function \( g \) via an efficient and intelligent method based on a set of discrete points

\[
\left\{ \left( O_i, C_{\text{Best}_O} \right) \right\} \subseteq \mathcal{O} \times \mathcal{C}_{\text{Best}_O}
\]  

generated by Eq. (5). In this way, Eq. (6) acquired will have high congruency with Eq. (5), and for this reason, it can be the final instruction of configuring the empirical coefficients according to the operating conditions.

3. COEFFICIENT ADAPTATION MODEL FOR THE ZWART MODEL

In the present study, we considered the coefficient adaptation problem of the Zwart model based on the simulation of the quasi-steady cavitating flows around a two-dimensional NACA66 (MOD) hydrofoil. The mathematical models \( M \) involved were the continuity, the momentum equation for the liquid-vapour mixture, the volume fraction equation for the liquid phase, the cavitation model, and the turbulence model. For simplicity, we focused only on the empirical coefficients of the cavitation model and neglected those of other equations. In 3.1, 3.2 and 3.3, the mathematical models related are introduced first, and in 3.4 the definition of the coefficient adaptation model for the Zwart model is given.
3.1 Governing Equations

In this study, the multiphase flow was solved via the homogeneous equilibrium approach:

\[
\frac{\partial \rho_{m}}{\partial t} + \frac{\partial \rho_{m} u_{j}}{\partial x_{j}} = 0
\]

(7)

\[
\frac{\partial \rho_{m} u_{j}}{\partial t} + \frac{\partial \rho_{m} u_{i} u_{j}}{\partial x_{j}} = -\frac{\partial \rho}{\partial x_{i}} + \frac{\partial}{\partial x_{j}} \left( \mu_{m} + \mu_{t} \right) \left( \frac{\partial u_{i}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{i}} \right)
\]

(8)

\[
\frac{\partial \rho_{m} \alpha_{i}}{\partial t} + \frac{\partial \rho_{m} \alpha_{i} u_{j}}{\partial x_{j}} = m^{+} + m^{-}
\]

(9)

The above equations are, in order, the continuity, the momentum equation for the liquid-vapour mixture, and the volume fraction equation for the liquid phase. Phases are considered incompressible and all phases share the same velocity field. \( u_{i} \) and \( u_{j}(m/s) \) represent the components of time-averaged mixture velocity, \( P(Pa) \) the time-averaged pressure, \( \rho_{m} \) the density of the liquid-vapour mixture, \( \rho_{l} \) the liquid density, \( \rho_{v} \) the vapour density, \( \alpha_{l} \) the liquid volume fraction, \( \alpha_{l} \) the vapour volume fraction, \( \alpha_{l} + \alpha_{v} = 1 \), \( \mu_{t} \) the dynamic viscosity of the liquid-vapour mixture, \( \mu \) the liquid dynamic viscosity, \( \mu_{t} \) the vapour density, \( \mu_{m} \) the turbulence viscosity, \( m^{+} \) the condensation rate, and \( m^{-} \) the evaporation rate. The density and the dynamic viscosity of the liquid-vapour mixture are defined as:

\[
\begin{aligned}
\rho_{m} &= \rho_{l} \alpha_{l} + \rho_{v} \alpha_{v} \\
\mu_{m} &= \mu_{l} \alpha_{l} + \mu_{v} \alpha_{v}
\end{aligned}
\]

(10)

In order to close the set of Eqs. (7),(8),(9), the turbulence viscosity \( \mu_{t} \) and the interphase mass transfer rate need to be modeled.

3.2 Turbulence Model

Cavitation flows are high Reynolds and high turbulent flows. In this study, the standard \( k - \varepsilon \) turbulence model was adopted. In the literature, the standard \( k - \varepsilon \) turbulence model performs well with simulating steady-state cavitation flows around the two-dimensional NACA66(MOD) hydrofoil. The transport equations of the turbulence kinetic energy \( k \) and the dissipation rate \( \varepsilon \) are as follows:

\[
\frac{\partial \rho k}{\partial t} + \frac{\partial \rho k u_{i}}{\partial x_{i}} = \frac{\partial}{\partial x_{i}} \left[ \mu_{m} + \frac{\mu_{t}}{\sigma_{k}} \right] \frac{\partial k}{\partial x_{i}}
\]

(11)

\[
\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho \varepsilon u_{i}}{\partial x_{i}} = C_{1e} \frac{\varepsilon}{k} \rho k \left[ 1 - C_{2e} \rho_{m} \varepsilon^{2} \right]
\]

(12)

where \( \mu_{t} \) represents the turbulent viscosity, \( \rho_{m} \) is the turbulent generation coefficient, \( C_{1e}, C_{2e}, \sigma_{k} \) and \( \sigma_{\varepsilon} \) are constants. \( \mu_{t} \) is calculated as below:

\[
\mu_{t} = \rho_{m} C_{\mu} \frac{k^{2}}{\varepsilon}
\]

(13)

where \( C_{\mu} \) is a constant. The values of the constants are as follows:

| Table 1 Constants of the standard \( k - \varepsilon \) model |
|-----------------|-----------------|-----------------|-----------------|
| \( C_{1e} \)    | \( C_{2e} \)    | \( C_{\mu} \)   | \( \sigma_{k} \) |
| 1.44            | 1.92            | 0.09            | 1.0             |
| 1.3             |                 |                 |                 |

To adapt to the Zwart model better, we modified \( \mu_{t} \) according to (Philip J. Zwart 2004):

\[
\mu_{t} = f(\rho) C_{\mu} \frac{k^{2}}{\varepsilon}
\]

(14)

Where

\[
f(\rho) = \rho_{l} + \left( \frac{\rho_{v} - \rho_{l}}{\rho_{v} - \rho_{l}} \right)^{n} \left( \rho_{l} - \rho_{v} \right)
\]

(15)

3.3 Cavitation Model

The cavitation model used in this study was the Zwart model, which was derived from a simplified Rayleigh – Plesset equation (Brennen 2005):

\[
m^{+} = F_{c} \frac{3 \alpha_{nuc} \rho_{l}}{R_{B}} \left[ \frac{2 P - P_{c}}{3 \rho_{l}} \right] \frac{2 P - P_{c}}{P_{c} - P_{v}} \rho_{v}
\]

(16)

\[
m^{-} = -F_{c} \frac{3 \alpha_{nuc} (1 - \alpha_{nuc}) \rho_{l}}{R_{B}} \left[ \frac{2 P - P_{c}}{3 \rho_{l}} \right] \rho_{v}
\]

(17)

where \( P_{v} \) is the saturated vapour pressure, \( \alpha_{nuc} \) is the nucleation site volume fraction, \( R_{B} \) is the radius of a nucleation site, \( F_{c} \) and \( F_{v} \) are two empirical coefficients for the condensation rate and the evaporation rate, respectively. In (Philip J. Zwart 2004), the default values of the above coefficients are given as: \( \alpha_{nuc} = 5 \times 10^{-4}, R_{B} = 1 \times 10^{-2}m, F_{c} = 0.01, F_{v} = 50 \). In literature, \( F_{c} \) and \( F_{v} \) are the calibration coefficients while the other two coefficients \( \alpha_{nuc} \) and \( R_{B} \) are set by default (Morgut, Nobile, Bilu, and Scaron 2011). In our study, we only considered \( F_{c} \) and \( F_{v} \), which directly control the cavitation process. Thus, \( C \) is expressed as \( C = (F_{c}, F_{v}) \). All the other coefficients are set with default values.

3.4 Definition of Coefficient Adaptation Model for the Zwart Model

The coefficient adaptation model for the Zwart model contains two key modules: the optimization module and the prediction module. The optimization module calibrates the empirical coefficients under limited number of operating
conditions and transfers the best values of the coefficients accompanied with the corresponding operating conditions to the prediction module, which will then model the relationship between the best values of the coefficients and the operating conditions. In the present study, we considered $O$ as a vector consisting of three components: the angle of attack $\alpha$ of the NACA66(MOD) hydrofoil, the inlet velocity $U_\infty$ and pressure $P_\infty$, namely $O = (\alpha, U_\infty, P_\infty)$. The objective function $f_O(C)$ was defined as the sum of the differences between the numerical values and the experimental values of the pressure coefficient, measured at 12 locations along the suction side of the NACA66(MOD) hydrofoil, for each couple of $C$ and $O$.

$$f_O(C) = \sum_{i=1}^{12} |C_{\text{P Sim}} - C_{\text{P Exp}}|$$  \hspace{1cm} (18)

In the above equation, $C_{\text{P Sim}}$ and $C_{\text{P Exp}}$ are the numerical value and the experimental value of the pressure coefficient at the $i$th location along the suction side of the hydrofoil under the operating condition $O$, respectively. $C_{\text{P Sim}}$ is calculated as:

$$C_{\text{P Sim}} = \frac{P_i - P_{\text{ref}}}{\frac{1}{2} \rho U_\infty^2}$$ \hspace{1cm} (19)

where $P_i$ is the numerical value of the local pressure at the $i$th location along the suction side of the hydrofoil, $P_{\text{ref}}$ is the reference pressure, and $\rho U_\infty^2$ is the theoretical pressure difference.

Assume that there is a set of limited number of operating conditions with corresponding experimental data $\Omega_{\text{Exp}} = \{O_1, \cdots, O_t\} \subset \Omega$. In the optimization module, all the elements in $\Omega_{\text{Exp}}$ are processed by Eqs. (18) and (5) in order to get the set of optimization results $E = \{(O_i, C_{\text{Best}i})|O_i \in \Omega, C_{\text{Best}i} \in \mathbb{C}, i = 1, \cdots, t\}$. We used $\text{Opt}(\cdot)$ as the function to represent the optimization process:

$$E = \text{Opt}(\Omega_{\text{Exp}}, C)$$ \hspace{1cm} (20)

Later, the prediction module will perform on $E$ to model the potential relationship between the best values of the coefficients $C = (F_c, F_e)$ and the operating conditions $O = (\alpha, U_\infty, P_\infty)$. Here, we neglected the interaction between $F_c$ and $F_e$, and separately considered their relationship with $\alpha$, $U_\infty$ and $P_\infty$. Let $M_{F_c}$ and $M_{F_e}$ be the relationship models related to the two coefficients $F_c$ and $F_e$ respectively. We used $\text{Train}(\cdot)$ as the function to represent the modeling process:

$$\left(M_{F_c}, M_{F_e}\right) = \text{Train}(E)$$ \hspace{1cm} (21)

Let $F_{\text{c Best}}$ and $F_{\text{e Best}}$ denote the best values of $F_c$ and $F_e$, which can be predicted by $M_{F_c}$ and $M_{F_e}$ respectively:

$$\begin{align*}
F_{\text{c Best}} &= M_1(\alpha, U_\infty, P_e) \\
F_{\text{e Best}} &= M_2(\alpha, U_\infty, P_e)
\end{align*}$$ \hspace{1cm} (22)

Equations (20) and (21) comprise the mathematical form of the coefficient adaptation model for the Zwart model. It should be noted that $M_{F_c}$ and $M_{F_e}$ can be trained and generated by different modeling methods, which can be treated as independent modules. In our study, we adopted one of the neural networks, the Radial Basis Function Neural Network (RBFNN) as the intelligent method to predict optimal coefficients. RBFNN has its outstanding advantages: It can approach any complicated nonlinear function relations and deal with the unanalyzable regularity in the system; It has good generalization ability and fast learning convergence speed. Thus, RBFNN has been successfully applied in time series analysis, pattern recognition, image processing, system modeling and other fields (Bellvin 2003; Lee and Ko 2009; Han, Chen, and Qiao 2011; Meng, Wu, Lu, and Toh 2002; Lu and Zhou 2009).

### 4. Design and Implementation of Coefficient Adaptation Method

As previously described, the coefficient adaptation model for the Zwart model contains the optimization module and the prediction module. The general framework is shown in Fig. 1. Firstly, the operating conditions and the corresponding experimental data are input to the whole system, and then the optimization module will generate an optimization case for each operating condition respectively. After that, the optimization module will create copies of the optimizer, which conducts the calibration of $F_c$ and $F_e$ for each optimization case. All the optimizers work in parallel and after all the optimization work is done, the optimization results will be collected and sent to the prediction module, which will build the relationship model to predict the optimal coefficients according to operating conditions.

The aim of coefficient optimization is to obtain the set of optimization results $E = \{(O_i, C_{\text{Best}i})|O_i \in \Omega, C_{\text{Best}i} \in \mathbb{C}, i = 1, \cdots, t\}$ for modeling use. The optimizer in the optimization module applies the surrogate-based sequential approximate optimization (SAO) method to acquire the best values of the empirical coefficients. The SAO method introduces the approximate model technique to the process of optimization and adopts an effective approach of renewing the sampling points, which can remarkably reduce time cost and resources. For this reason, it has been widely used in complex engineering optimization. (Queipo, Haftka, Wei, Goel, Vaidyanathan, and Tucker 2005; Kleijnen 1986; Forrester and Keane 2009). We implemented the SAO method specifically for our research goal. The SAO method mainly consists of three parts: preconditioning, approximate modeling and renewing of sampling points. The process of the SAO method is shown in Fig. 2.

Preconditioning deals with the scale unification between the two design variables $F_c$ and $F_e$, the...
selection of the initial sampling points, namely the initial values of the design variables, and simulation at the sampling points, the aim of which is to calculate the values of the objective function based on numerical results and to prepare for the approximate modeling. We applied the Optimal Latin Hypercube Design (OLHD) method to conduct the optimal selection of the initial sampling points within the design space (Park 1994). The design space is expanded referring to (Morgut, Nobile, Bilu, and Scaron 2011):

\[
\begin{align*}
F_c &= [0.0001, 0.1] \\
F_e &= [5,1000]
\end{align*}
\] (23)

Approximate modeling builds a surrogate model using fitting and interpolation based on radical basis function network (Thomspson and Alexandra 1996) to predict the optimal values of \(F_c\) and \(F_e\) which combine to minimize the objective function. In order to validate the surrogate model, simulation will be performed with the predicted values of the coefficients to acquire the numerical results that can be used to calculate the objective function. If deviation between the calculated values and the predicted values of the objective function is undesirable, then the surrogate model will be reconstructed. Above steps will be repeated until the desirable surrogate model and the corresponding optimal values of the coefficients are found. Renewing of sampling points helps with the reconstruction of the surrogate model by adding a sampling point for building the surrogate model, using a Pareto front sampling method (Hughes 2003) to determine the new sampling point. The termination criteria is used to terminate the algorithm iteration process. A high-efficiency convergence criteria can drastically reduce unnecessary computational consumption. In our study, the two-step termination criteria was applied (Wang, Hu, Ma, Wu, and Zhang 2014):

1. If the new sampling point no longer contributes to the surrogate model updating.
2. If the new sampling point no longer contributes to the performance of the surrogate model at the optimal point.

The implementation of SAO approach was validated by solving Eq. (24) mentioned in (Wang, Hu, Ma, Wu, and Zhang 2014) before allocated into the optimizer. The evaluation results were similar to those given by (Wang, Hu, Ma, Wu, and Zhang 2014), which proved the effectiveness and efficiency of the implementation.

\[
\begin{align*}
\min f(x) &= (4 - 2.1x_1^2 + \frac{x_1^4}{3})x_1^2 + x_1x_2 \\
&+ (4x_2^2 - 4)x_2 + x_1 + x_2 \\
-2 &\leq x_1, x_2 \leq 2
\end{align*}
\] (24)

The optimizer will output the operating condition and the corresponding best values of the empirical coefficients after the iteration process terminates. Finally the prediction module will invoke the RBFNN module to build the relationship model after receiving the set of optimization results.

5. VALIDATION AND EVALUATION

5.1 Platform

Our tests were carried out on a HPC cluster situated in the State Key Laboratory of High Performance Computing, China. This hardware platform consists of hundreds of computing nodes connected via InfiniBand network with a total bandwidth of 40 Gb/s, and each computing node contains two hexacore 2.1 GHz Intel Xeon E5-2620 CPUs and 16 GB memory. The operating system of the cluster is Red Hat Enterprise Linux Server 6.5, on which OpenFOAM version 2.3.1 is installed. OpenFOAM
is an open source software for CFD which allows user-defined solvers and has good parallel computing capability. The solver used in our study was the interPhaseChangeFoam, which can solve multiphase flows. Because the interPhaseChangeFoam hasn’t included the Zwart model, we programmed the Zwart model first and then implemented the coefficient adaptation platform for the Zwart model combined with OpenFOAM. In the prediction module, we invoked the RBNN tools from MATLAB software to model the relationship between the optimal coefficients and the operating conditions.

5.2 Mesh and Case Setup

In the present study we considered the NACA66(MOD) hydrofoil with a camber ratio of $f/c = 0.20$, a NACA meanline of $a = 0.8$ and a thickness ratio of $t/c = 0.9$, where $f$ is the maximum thickness, $t$ the maximum camber and $c$ the chord length of the hydrofoil section. The experimental data was from the measurements carried out by Shen and Dimotakis et al. in the High-Speed Water Tunnel of the California Institute of Technology (Dimotakis, Gaebler, Hamaguchi, Lang, and Shen 1987). In their experiments, the chord length of the hydrofoil model was $c = 0.150m$. During the experiments, leading edge sheet cavitation and midchord cavitation were investigated with the hydrofoil model placed at several angles of attack. In our study, we chose all the cases (28 in total) with definite experimental results under different combinations of the angle of attack $\alpha$, the inflow velocity $U_\infty$ and the inflow pressure $P_\infty$.

Rectangular domains were used in order to simulate the flows around the hydrofoil at different angles of attack. All the meshes were hexa-structured and generated using the ANSYS ICEM CFD 17.0 tool. It should be emphasized that although OpenFOAM can simulate two-dimensional flows, it can only support three-dimensional meshes. The original two-dimensional meshes from ICEM were converted to three-dimensional ones with small thickness by OpenFOAM’s built-in tools. The boundary type of the additional two faces (Front and Back) of the three-dimensional meshes was set to “empty” in OpenFOAM, in order to achieve two-dimensional simulations. The computational domain and the imposed boundary conditions are shown in Fig. 3. The meshes were set as follows:

1. The Inlet and Outlet boundaries were placed respectively 3 chord lengths ahead of the leading edge, and 5 chord lengths behind the trailing edge. The Top and Bottom boundaries were placed 2.5 chord lengths from the hydrofoil.

2. Average values of $y'$ on the hydrofoil surfaces were 30. $y'$ was defined as $y' = (\mu v)/\nu$ where $\mu$ is the friction velocity, $v$ the normal distance from the wall, $\nu$ the kinematic viscosity.

3. On solid surfaces (Top, Bottom, Hydrofoil) the no-slip condition was applied.

4. The type of Front and Back boundaries was set to “empty” in OpenFOAM.

Before operating on the coefficient adaptation platform, the study of the influence of the mesh resolution was carried out in fully wetted (non-cavitating) conditions. This investigation was performed on the hydrofoils at all the angles of attack concerned in our study, by monitoring the influence of the progressively finer meshes on the lift coefficient $C_L$ and the drag coefficient $C_D$. During the mesh refinement, the distances of the first nodes from the solid surfaces were kept unchanged, in order to perform a consistent mesh independence study. 48 processes for parallel simulation were allocated, which was also configured in the optimization module. $C_L$ and $C_D$ are defined as follows:

$$C_L = \frac{F_L}{(1/2) \rho U_\infty^2 S} \quad C_D = \frac{F_D}{(1/2) \rho U_\infty^2 S}$$

(25)

where $S = c \times d$ is the planar surface with $d$ equal to the span. The span in our study was set to $d = 0.01m$, which was the same as the thickness of the meshes.

Table 2 Results of the mesh independence study carried out for NACA66(MOD) at $\alpha = 4^\circ$ and $Re = 2 \times 10^6$.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Nodes</th>
<th>$C_L$</th>
<th>$C_D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>41788</td>
<td>0.652</td>
<td>0.0017</td>
</tr>
<tr>
<td>Mid</td>
<td>97123</td>
<td>0.654</td>
<td>0.0018</td>
</tr>
<tr>
<td>Fine</td>
<td>186433</td>
<td>0.647</td>
<td>0.0019</td>
</tr>
<tr>
<td>Exp.</td>
<td>0.629</td>
<td>0.0018</td>
<td></td>
</tr>
</tbody>
</table>

Simulations under fully wetted conditions were conducted for all the angles of attack. Take the hydrofoil at $\alpha = 4^\circ$ as an example. The value of the free-stream velocity on the Inlet boundary was set to $U_\infty = 12.2m/s(Re = 2 \times 10^6)$ and the value of the static pressure on the Outlet boundary was set to 202650Pa. Table 2 shows the results of the mesh independence study. From
In simulating cavitating flows, we had, for each case and the corresponding computational mesh, the following settings besides those mentioned in mesh resolution study:

1. The value of the free-stream velocity on the Inlet boundary and the value of the static pressure on the Outlet boundary were set respectively equal to the $U_\infty$ and $P_\infty$ corresponding to each case. Initial water and vapour volume fractions were set to 1 and 0, respectively.

2. In all the simulations the water and vapour density were kept constant and equal to $\rho_w = 997 \text{kg/m}^3$ and $\rho_v = 0.02308 \text{kg/m}^3$. Assuming a turbulence intensity of 1%, the turbulent kinetic energy $k$ and the turbulent dissipation rate $\varepsilon$ were set equal to $k = 0.0233 \text{m}^2/\text{s}^2$ and $\varepsilon = 0.1837 \text{m}^2/\text{s}^3$. The saturated vapour pressure of water was $P_v = 3169 \text{Pa}$.

5.3 Implementary Methodology

The aim of our tests was to validate the coefficient adaptation method for the Zwart model. After receiving the input of the operating conditions and experimental data of the 28 cases, the coefficient adaptation platform will generate and configure optimization cases on OpenFOAM as mentioned in 5.2, and activate the optimization module to perform parallel optimization work, whose results will be sent to the prediction module. In the prediction module, the optimization results of 3/4 of the cases were chosen randomly (covering all the angles of attack) as the training set to build the relationship model. The rest 1/4 cases (which will be called the test cases from now on) were used for subsequent validation of the model. For each test case, the best values of the coefficients $C_{\text{predicted}} = \{F_{\text{predicted}}, \ldots\}$ with $O_i = (\alpha_i, U_{\alpha_i}, P_{\alpha_i})$ $(i = 1, \ldots, 7)$ according to the relationship model were predicted.

We used the following equation to evaluate the predicted values of the coefficients:

$$Err_{\text{predicted}} = \frac{1}{7} \sum_{i=1}^{7} f_i \left( C_{\text{predicted}} - f_i(C_{\text{Best}}) \right)$$

(26)

The smaller $Err_{\text{predicted}}$ is the closer to the best simulation results, thus the more consistent with the experimental data. Moreover, we tested the default values in (Philip J. Zwart 2004) and the tuned values in (Morgut, Nobile, Bilu, and Scaron 2011).

We replaced $C_{\text{predicted}}$ in Eq. (26) with $C_{\text{Default}} = (0.01, 50)$ and $C_{\text{Morgut}} = (0.03, 300)$ respectively, and compared the results $Err_{\text{Default}}$ and $Err_{\text{Morgut}}$ with $Err_{\text{Predicted}}$.

5.4 Results and Discussion

The optimization results of the 28 cases yielded from the optimization module are shown in Table 3. $C_{\text{Best}} = (F_{\text{Best}}, F_{\text{Best}})$ denotes the best values of the empirical coefficients. The cavitation number $\sigma$ in Table 3 is calculated as:

$$\sigma = \frac{P_v - P_\alpha}{\frac{1}{2} \rho_w U_\infty^2}$$

(27)

The number of iterations and mean CPU time in the SAO approach for each case are shown in Fig. 6. It is possible to see the efficiency and stable performance of the SAO approach from the figure. In this study, the number of iterations went from 5 to 15. It presents similar level of efficiency to the literature (Wang, Hu, Ma, Wu, and Zhang 2014). By allocating 48 processes for simulation during each single iteration, the mean CPU time was kept in the range of 6000 to 9000 seconds. The optimization results were collected after all the cases were done, and thus there would be a waste of waiting time. As the iterations and mean CPU time among the cases were relatively close, the waiting
time was acceptable compared to the total CPU time cost in the optimization module. An example of the iterative convergence is demonstrated in Fig. 7. It presents the convergence curve of the objective function in Case 15. As is shown in the figure, the minimum of the objective function, which corresponds to the optimal values of the empirical coefficients, is found after 144 iterations. Moreover, the accuracy of the optimization approach can be seen in Figs. 8 and 9, by comparing the best simulation results with the experimental data.

21 sets of optimization results were randomly chosen (covering all the angles of attack) as the input to the RBFNN (labeled M in Table 3) to build the relationship model. The predicted optimal coefficients by the relationship model $C_{\text{predicted}} = \ldots$
Fig. 5. Mid resolution mesh around NACA66(MOD) at the angle of attack of $\alpha=4^\circ$; large view(left), close view(right).

Fig. 6. Number of iterations (bottom) and mean CPU time (top) in the SAO approach for each case. The dash lines represent the average of the number of iterations and the average of the mean CPU time, respectively.

$(F_{c,\text{Predicted}}, F_{e,\text{Predicted}})$ of the 7 test cases (labeled V in Table 3) are shown in Table 4. For each test case, simulations with $C_{\text{Best}}, C_{\text{Default}}, C_{\text{Morgut}}$ and $C_{\text{Predicted}}$ respectively were carried out. With the simulation results we calculated the corresponding values of the objective function $f(C)$, as shown in Table 5. Preliminarily we can see the predicted values are better than the default values and the Morgut values in overall.

Table 4 Predicted values of $F_c$ and $F_e$ for the test cases. The number of the case is in agreement with Table 3

<table>
<thead>
<tr>
<th>No.</th>
<th>$\sigma$</th>
<th>$\alpha(\circ)$</th>
<th>$F_{c,\text{Predicted}}$</th>
<th>$F_{e,\text{Predicted}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.42</td>
<td>1</td>
<td>0.0717</td>
<td>866.41</td>
</tr>
<tr>
<td>7</td>
<td>0.55</td>
<td>2</td>
<td>0.0433</td>
<td>618.65</td>
</tr>
<tr>
<td>13</td>
<td>1.12</td>
<td>4</td>
<td>0.0763</td>
<td>878.00</td>
</tr>
<tr>
<td>15</td>
<td>0.91</td>
<td>4</td>
<td>0.0702</td>
<td>809.41</td>
</tr>
<tr>
<td>19</td>
<td>0.94</td>
<td>4</td>
<td>0.0459</td>
<td>644.57</td>
</tr>
<tr>
<td>25</td>
<td>1.48</td>
<td>6</td>
<td>0.0699</td>
<td>701.28</td>
</tr>
<tr>
<td>28</td>
<td>0.98</td>
<td>6</td>
<td>0.0647</td>
<td>656.97</td>
</tr>
</tbody>
</table>

Table 5 Objective function calculated from the simulation results of the test cases with respectively four pairs of empirical coefficients

<table>
<thead>
<tr>
<th>No.</th>
<th>Best</th>
<th>Default</th>
<th>Morgut</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.764</td>
<td>0.774</td>
<td>0.785</td>
<td>0.787</td>
</tr>
<tr>
<td>7</td>
<td>0.124</td>
<td>0.237</td>
<td>0.238</td>
<td>0.157</td>
</tr>
<tr>
<td>13</td>
<td>0.188</td>
<td>0.237</td>
<td>0.238</td>
<td>0.206</td>
</tr>
<tr>
<td>15</td>
<td>0.285</td>
<td>0.298</td>
<td>0.302</td>
<td>0.293</td>
</tr>
<tr>
<td>19</td>
<td>0.282</td>
<td>0.309</td>
<td>0.301</td>
<td>0.298</td>
</tr>
<tr>
<td>25</td>
<td>0.477</td>
<td>0.499</td>
<td>0.493</td>
<td>0.499</td>
</tr>
<tr>
<td>28</td>
<td>1.238</td>
<td>1.292</td>
<td>1.284</td>
<td>1.239</td>
</tr>
</tbody>
</table>

Further observation of the pressure distributions along the surface of the hydrofoil is demonstrated in Fig. 8, and the cavitation patterns in Fig. 9. From the results given in Fig. 8, it seems that the pressure distributions along the pressure side (the lower lines) computed from different pairs of coefficient values are quite close to each other, but the suction side pressure distributions are obviously different. It can be concluded that the condensation and the
evaporation coefficients mainly influence the low-pressure area where cavitation occurs. In Case 2, midchord cavitation is observed over the hydrofoil at $\alpha = 1^\circ$, and that the lengths of cavity obtained with $C_{\text{Default}}$, $C_{\text{Morgut}}$ and $C_{\text{Predicted}}$ are close to one another and are all much larger than that obtained with $C_{\text{Best}}$. It should be noted that even the best simulation results differ much from the experimental measurements. In Case 7 leading edge sheet cavitation at $\alpha = 2^\circ$ is shown. Compared with $C_{\text{Default}}$ and $C_{\text{Morgut}}$, the cavity length obtained with $C_{\text{Predicted}}$ is shorter and closer to that obtained with $C_{\text{Best}}$, and the suction side pressure coefficients are in better agreement with experimental measurements. Case 11, 15, and 19 show leading edge cavitation at $\alpha = 4^\circ$. In Case 11 the effects of all the pairs of coefficients are quite similar and agree well with the experimental measurements. In Case 15 the cavity length obtained with $C_{\text{Predicted}}$ is smaller and the suction side distributions agree better with experimental measurements, compared with $C_{\text{Default}}$ or $C_{\text{Morgut}}$. In Case 19, all the pairs of empirical coefficients have almost the same effect on the cavity pattern and the suction side pressure coefficients, with a small difference in the prediction of pressure at the end of the cavity. Case 25 and 28 show leading edge sheet cavitation at $\alpha = 6^\circ$. In Case 25 compared with $C_{\text{Default}}$ and $C_{\text{Morgut}}$, the cavity length obtained with $C_{\text{Predicted}}$ is closer to experimental measurements, but the prediction of pressure at the end of the cavity is less accurate. In Case 28 the effects of all the pairs of coefficients differ much from the experimental measurements, but we still can see $C_{\text{Predicted}}$ performs better than $C_{\text{Default}}$ or $C_{\text{Morgut}}$. In general, we can conclude that $C_{\text{Predicted}}$ is better than $C_{\text{Default}}$ and $C_{\text{Morgut}}$.

![Fig. 7. Iterative convergence curve of the objective function of Case 15.](image)

**Fig. 7. Iterative convergence curve of the objective function of Case 15.**

**Table 6 Evaluation of $C_{\text{Default}}$, $C_{\text{Morgut}}$ and $C_{\text{Predicted}}$**

<table>
<thead>
<tr>
<th>$\text{Err}_{\text{Default}}$</th>
<th>$\text{Err}_{\text{Morgut}}$</th>
<th>$\text{Err}_{\text{Predicted}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.318</td>
<td>0.319</td>
<td>0.194</td>
</tr>
</tbody>
</table>

With Table 5 $\text{Err}_{\text{Default}}$, $\text{Err}_{\text{Morgut}}$ and $\text{Err}_{\text{Predicted}}$ were calculated, as shown in Table 6. We can see $\text{Err}_{\text{Default}}$ and $\text{Err}_{\text{Morgut}}$ are quite close to each other, indicating that the default values of the empirical coefficients result in similar accuracy with the Morgut values. Moreover, compared with the constant values, that is, the default values and the Morgut values, the predicted values of the empirical coefficients increase the simulation accuracy by about 12% in average.

The overall results indicate that it is effective to use the coefficient adaptation method to solve the coefficient adaptation problem for the Zwart model and guide the configuration of the empirical coefficients under different operating conditions.

### 6. CONCLUSION

The coefficient adaptation problem is often encountered in CFD simulations. The accuracy of the simulation results depends much on the empirical coefficients of mathematical models. In literature, constant values of empirical coefficients are applied regardless of the operating conditions, and thus they cannot meet the needs of all operating conditions with good performance. Cavitation simulation is a typical application of CFD. Many modeling methods have been proposed to simulate cavitating flows in many cases. A widely used method is to solve RANS (Reynolds Averaged Navier Stokes) equations with an additional transport equation including the cavitation model which describes the variation of the volume fraction of the liquid phase. In cavitation simulations, researchers have proposed methods of obtaining the best values of the empirical coefficients of the cavitation model. However, these methods can only acquire constant values which aren’t adaptive to all the operating conditions. In our present study, we focused on the Zwart model and carried out research into the prediction of the best values of empirical coefficients, considering quasi-steady cavitating flows around a two-dimensional NACA66(MOD) hydrofoil. The main contributions of this paper are summarized as follows:

1. For the first time, we gave a formal description of the coefficient adaptation problem and solution, and put forward the coefficient adaptation model and corresponding method including two key modules: the optimization module and the prediction module, which could model the relationship between the optimal coefficients of the CFD model and the operating conditions based on existed experimental measurements.

2. We designed and implemented the coefficient adaptation platform for the Zwart model through the method mentioned above, combining the open source software OpenFOAM. Then we performed optimization of the condensation coefficient $F_{c}$ and the evaporation coefficient $F_{e}$ of the Zwart model and validated the predicted optimal coefficients on the platform.

3. The overall results indicate that our method can effectively solve the coefficient adaptation problem of the Zwart model. The predicted coefficient values result in an
Fig. 8. Comparison of pressure distributions along the suction side (the upper lines) and the pressure side (the lower lines) of the NACA66(MOD) hydrofoil resulting from different pairs of empirical coefficients in the test cases.

Fig. 9. Cavitation patterns resulting from different pairs of empirical coefficients (in order $C_{\text{Default}}$, $C_{\text{Morgut}}$, $C_{\text{Predicted}}$ and $C_{\text{Best}}$) in the test cases. The color scale shows different values of water volume fraction $\alpha_l$. 
increase of accuracy by 12% in average, compared with the default values (Philip J. Zwart 2004) and the tuned values given in (Morgut, Nobile, Bilu, and Scaron 2011).

We believe that the proposed method could be very useful in adaptively configuring the empirical coefficients of present, and also future, mathematical models in practical uses.

ACKNOWLEDGMENTS

The authors declare that there is no conflict of interest regarding the publication of this paper. The authors would like to thank the Key Research and Development Plan of Ministry of Science and Technology (Grant no. 2016YFB0201301) and the Science Challenge Program of CAEP (no. JCKY2016212A502 and TZ2016002) for funding.

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